

Fast approximate furthest neighbors with data-dependent hashing

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Abstract. We present a novel hashing strategy for approximate furthest neighbor search that selects projection bases using the data distribution. This strategy leads to an algorithm, which we call **DrusillaHash**, that is able to outperform existing approximate furthest neighbor strategies. Our strategy is motivated by an empirical study of the behavior of the furthest neighbor search problem, which lends intuition for where our algorithm is most useful. We also present a variant of the algorithm that gives an absolute approximation guarantee; to our knowledge, this is the first such approximate furthest neighbor hashing approach to give such a guarantee. Performance studies indicate that **DrusillaHash** can achieve comparable levels of approximation to other algorithms while giving up to an order of magnitude speedup. An implementation is available in the **mlpack** machine learning library (found at <http://www.mlpack.org>).

1 Introduction

We concern ourselves with the problem of *furthest neighbor search*, which is the logical opposite of the well-known problem of nearest neighbor search. Instead of finding the nearest neighbor of a query point, our goal is to find the furthest neighbor. This problem has applications in recommender systems, where furthest neighbors can increase the diversity of recommendations [1,2]. Furthest neighbor search is also a component in some nonlinear dimensionality reduction algorithms [3], complete linkage clustering [4,5] and other clustering applications [6]. Thus, being able to quickly return furthest neighbors is a significant practical concern for many applications.

However, it is in general not feasible to return exact furthest neighbors from large sets of points. Although this is possible with Voronoi diagrams in 2 or 3 dimensions [7], and with single-tree or dual-tree algorithms in higher dimensions [8], these algorithms tend to have long running times in practice. Therefore, approximate algorithms are often considered acceptable in most applications.

For approximate neighbor search algorithms, hashing strategies are a popular option [9,10,11]. Typically hashing has been applied to the problem of nearest neighbor search, but recently there has been interest in applying hashing techniques to furthest neighbor search [12,13]. In general, these techniques are

based on random projections, where random unit vectors are chosen as projection bases. This allows probabilistic error guarantees, but the entirely random approach does not use the structure of the dataset.

In this paper, we first consider the structure of the furthest neighbors problem and then conclude that a data-dependent approach can be used to select the projection bases for a hashing algorithm. This allows us to develop:

- **DrusillaHash**, a hashing algorithm that uses data-dependent projection bases and outperforms other approximate furthest neighbors approaches in practice.
- A modified version of **DrusillaHash** which satisfies rigorous approximation guarantees, though it is not likely to be useful in practice.

Our empirical results in Section 7 show that the **DrusillaHash** algorithm demonstrably outperforms existing solutions for approximate k -furthest-neighbor search.

2 Notation and formal problem description

The problem of furthest neighbor search is easily formalized. Given a set of *reference points* $S_r \in \mathcal{R}^{n \times d}$, a set of *query points* $S_q \in \mathcal{R}^{m \times d}$, and a distance metric $d(\cdot, \cdot)$, the problem is to find, for each query point $p_q \in S_q$,

$$\operatorname{argmax}_{p_r \in S_r} d(p_q, p_r). \quad (1)$$

A trivial way to solve this algorithm is by brute-force: for each query point, loop over all reference points and find the furthest one. But this algorithm takes $O(nm)$ time, and does not scale well to large S_r or S_q . In this paper, we will consider the ϵ -approximate form of the furthest neighbor search problem.

Given a set of *reference points* $S_r \in \mathcal{R}^{n \times d}$, a set of *query points* $S_q \in \mathcal{R}^{m \times d}$, an approximation parameter $\epsilon \geq 0$, and a distance metric $d(\cdot, \cdot)$, the ϵ -approximate furthest neighbor problem is to find a furthest neighbor candidate \hat{p}_{fn} for each query point $p_q \in S_q$ such that

$$\frac{d(p_q, p_{fn})}{d(p_q, \hat{p}_{fn})} < 1 + \epsilon \quad (2)$$

where p_{fn} is the true furthest neighbor of p_q in S_r . When $\epsilon = 0$, this reduces to the exact furthest neighbor search problem. This form of approximation is also known as relative-value approximation.

3 Related work

There have been a number of improvements over the naive brute-force search algorithm suggested above. Exact techniques based on Voronoi diagrams can solve the furthest neighbor problem. In 1981, Toussaint and Bhattacharya proposed building a furthest-point Voronoi diagram to solve the furthest neighbors problem in $O(m \log n)$ time [14]. But in high dimensions, Voronoi diagrams are not useful because of their exponential memory dependence on the dimension.

Another approach to exact furthest neighbor search uses space trees, as described by Curtin et al. [8]. A tree is built on the reference points S_r , and nodes that cannot contain the furthest neighbor of a given query point are pruned. This is essentially equivalent to many algorithms for nearest neighbor search, such as the algorithm for nearest neighbor search with cover trees [15], but with inequalities reversed (i.e., we prune nearby nodes instead of faraway nodes). It is also possible to do this in a dual-tree setting, by also building a tree on the query points S_q . Dual-tree nearest neighbor search has been proven to scale linearly in the size of the reference set under some conditions [16]; however, no similar bound has been shown for dual-tree furthest neighbor search. It would be reasonable to expect similar empirical scaling. Unfortunately, tree-based approaches tend to perform poorly in high dimensions, and the construction time of the trees can cause the algorithm to be slower than desirable in practice.

Further runtime acceleration can be achieved if approximation is allowed. It is easy to modify the single-tree and dual-tree algorithms to support this, in the manner suggested by Curtin for nearest neighbor search [17]. Although this is shown to accelerate nearest neighbor search runtime by a significant amount (depending on the allowed approximation), the setup time of building the trees can still dominate. A similar approach to this strategy is the fair split tree, designed by Bespamyatnikh [18]. But this approach suffers from the same issues.

The fastest known algorithms for approximate nearest neighbor search are hashing algorithms. Indyk [13] proposed a hashing algorithm based on random projections that is able to solve a slightly different problem: this algorithm is able to determine (approximately) whether or not there exists a point in S_r farther away than a given distance. This can be reduced to the approximate furthest neighbor problem we are interested in, but this is complex to implement.

Pagh et al. [12] refine this approach in order to directly solve the approximate furthest neighbor problem; this improves on the runtime of Indyk’s algorithm and is easy to implement. This algorithm, called QDAFN (‘query-dependent approximate furthest neighbor’), has a guaranteed success probability. The algorithm is parameterized by the number of projections used and the number of points stored for each projection; usually, this number is relatively low. But in extremely high-dimensional settings, the randomly-chosen projections can fail to capture important outlying points. This motivates us to investigate the point distribution in order to choose projection bases.

4 Furthest neighbor point distribution

The furthest neighbor problem is significantly different from the nearest neighbor problem, which has received significantly more attention [19,20,21,22,9,8,17]. This difference is perhaps somewhat counterintuitive, given that the furthest neighbor problem is simply an argmax over all reference points instead of an argmin. But this small change causes the problem to have surprisingly different structure with respect to the results.

As a first observation of the differences between the two problems, consider that for any set S_r , the furthest neighbor of every point can be made to be a

single point simply by adding a single point sufficiently far from every other point in S_r . There is no analog to this in the nearest neighbor search problem. Indeed, it is often true that for a furthest neighbor query with many query points, the results may contain the same reference point. This is easily demonstrated.

Define the **rank** of a reference point p_r for some query point p_q as the position of p_r in the ordered list of distances from p_q . That is, if the rank of p_r for some query point p_q is k , then p_r is the k -furthest neighbor from p_q .

We can obtain insight into the behavior of furthest neighbor queries by observing the average rank of points on some example datasets from the UCI dataset repository [23]. Figure 1 contains scatterplots displaying the average rank of a reference point versus the mean-centered norm of the reference point for the all-furthest-neighbors problem (that is, each point in the reference set is used as a query point).

Figure 1 shows that there is a clear and unmistakable correlation between the norm of a point and its average rank for the all- k -furthest-neighbor problem. For the **ozone** dataset, we can see that there are only a few points with high norm, and all of these have much lower average rank than the rest of the points.

These observations suggest that a reasonable approximate furthest neighbor algorithm might be obtained simply by searching over the top few points in the reference set with highest norm. Unfortunately, an algorithm that simple will fail in many cases in practice. Still, an effective furthest neighbors algorithm

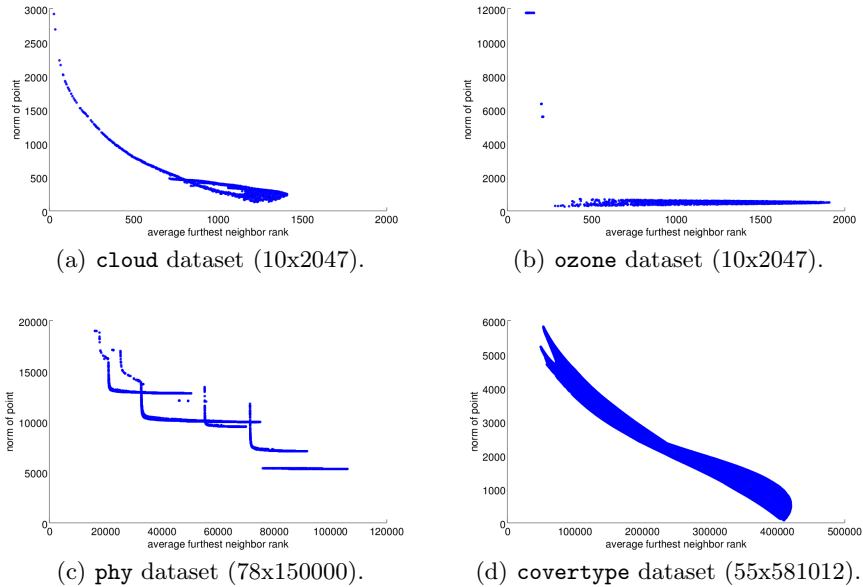


Fig. 1. Average rank vs. norm for a handful of datasets. Observe that a large norm is correlated with a low rank.

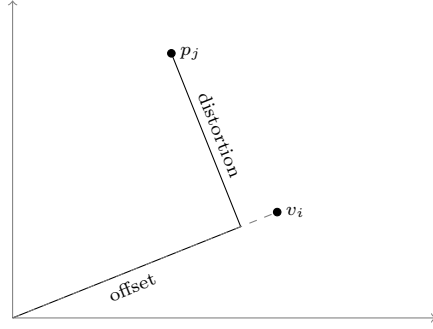


Fig. 2. Distortion and offset for p_j with base vector v_i .

should take this structure into account: *high-norm points are more important than low-norm points.*

5 The algorithm: DrusillaHash

Our collective observations motivate a hashing algorithm for approximate furthest neighbor search, which we introduce as **DrusillaHash** in Algorithm 1. The algorithm constructs hash tables by repeatedly choosing points currently not in any hash table with largest norm.¹ After the hash tables are built, each query point is simply compared with all points in each hash table in order to determine a good furthest neighbor candidate.

DrusillaHash depends on two parameters: l , the number of tables, and m , the number of points taken for each table. Empirically we observe that values in the range of $l \in [2, 15]$ and $m \in [1, 5]$ produce acceptably good approximations for most datasets, with approximation levels between $\epsilon = 0.01$ and $\epsilon = 1.1$.

The primary intuition of the algorithm is that we want to collect points in the hash tables R_i that are likely to be furthest neighbors of any query point. We know from our earlier experiments that points with high mean-centered norms are likely to be good furthest neighbor candidates. Thus, we start by selecting the highest-norm mean-centered point p_i as the primary point of the table R_i , and collect m points that are not too distorted by a projection onto the unit vector v_i which points in the direction of p_i . Any points that are not too distorted by this projection but not collected are ignored for future tables (line 22).

The words “not too distorted” deserve some elaboration: we wish to find high-norm points that are well-represented by p_i , but we do not wish to find high-norm points that are *not* well-represented by p_i . Ideally, those points will be selected as the primary point of another table R_j . Therefore, for each point p_j , we calculate the offset $O[p_j]$; this is the norm of the projection of p_j onto v_i . Similarly, we calculate the distortion $D[p_j]$. Figure 2 displays a simple example of offset and distortion.

¹ This is where the algorithm gets its name; the first author’s cat displays the same behavior when selecting a food bowl to eat from.

Algorithm 1 DrusillaHash: fast approximate k -furthest neighbor search.

```
1: Input: reference set  $S_r$ , query set  $S_q$ , number of neighbors  $k$ , number of tables  $l$ ,  
   table size  $m$   
2: Output: array of furthest neighbors  $N[]$   
3: {Pre-processing: mean-center data.}  
4:  $m \leftarrow \frac{1}{n} \sum_{p_r \in S_r} p_r$   
5:  $S_r \leftarrow S_r - m$ ;  $S_q \leftarrow S_q - m$   
  
6: {Pre-processing: build DrusillaHash tables.}  
7:  $V \leftarrow \{\}$   
8: for all  $p_r \in S_r$  do  $n[p_r] \leftarrow \|p_r\|$  {Initialize norms of points.}  
9: for all  $i \in \{0, 1, \dots, l\}$  do  
10:   $p_i \leftarrow \operatorname{argmax}_{p_r \in S_r} n[p_r]$  {Take next point with largest norm.}  
11:   $v_i \leftarrow p_i / \|p_i\|$   
12:   $V \leftarrow V \cup \{v_i\}$   
  
13: {Calculate distortions and offsets.}  
14: for all  $p_r \in S_r$  such that  $n[p_r] \neq 0$  do  
15:    $O[p_r] \leftarrow p_r^T v_i$   
16:    $D[p_r] \leftarrow \|p_r - O[p_r]v_i\|$   
17:    $s[p_r] \leftarrow |O[p_r]| - D[p_r]$   
  
18: {Collect points that are well-represented by  $p_i$ .}  
19:  $R_i \leftarrow$  points corresponding to largest  $m$  elements of  $s[\cdot]$   
20: for all  $p_r \in R_i$  do  $n[p_r] = 0$  {Mark point as used.}  
21: for all  $p_r \in S_r$  such that  $\operatorname{atan}(D[p_r]/O[p_r]) \geq \pi/8$  do  
22:    $n[p_r] = 0$  {Mark point as used.}  
  
23: {Search for furthest neighbors.}  
24: for all  $p_q \in S_q$  do  
25:   for all  $R_i \in R$  do  
26:     for all  $p_r \in R_i$  do  
27:       if  $d(p_q, p_r) > N_k[p_q]$  then  
28:         update results  $N[p_q]$  for  $p_q$  with  $p_r$ 
```

Our goal is to balance two objectives in selecting points for R_i :

- Select high-norm points.
- Select points that are well-represented by v_i .

The solution we have used here is to construct a score $s[p_j]$ which is just the distortion subtracted from the offset (see line 17). Figure 3 displays an example v_i with 20 points; each point is indexed by its position in the ordered score set $s[\cdot]$. In the context of DrusillaHash, if we took $m = 6$ (so, 6 points were selected for each v_i), then v_i and the five red points p_1 through p_5 would be selected to make up the table R_i . Then, p_7 would be chosen as v_{i+1} because it is the point with largest norm that has not been selected to be in a hash table (line 10).

Once we have constructed the tables R_i , then our actual search is a simple brute-force search over every point contained in each table R_i . Because the total number of points in R is only lm , brute-force scan is sufficient. In our experiments, attempting to prune points in R involved too much overhead.

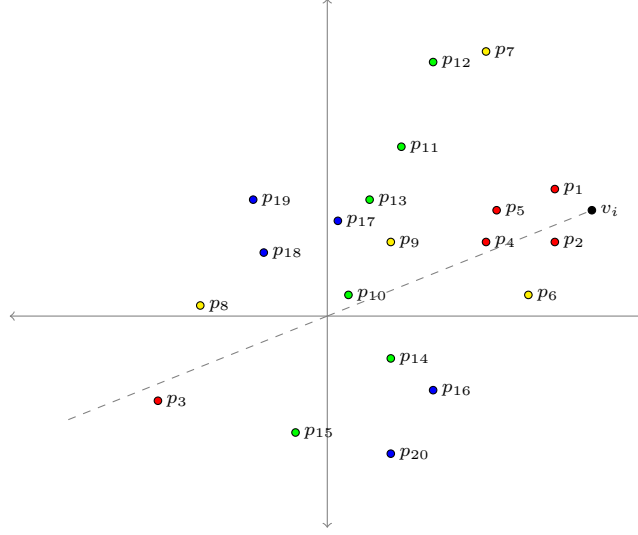


Fig. 3. Example scores for a set of points; red: highest scores, blue: lowest scores.

Algorithm	Setup time	Search time
DrusillaHash	$O(ld S_r \log S_r)$	$O(S_q dlm)$
QDAFN [12]	$O(ld S_r \log S_r)$	$O(S_q d(l \log l + m \log l))$
Indyk [13]	$O(ld S_r \log S_r)$	$O(l S_q (d + \log S_r) \log d \log \log d)$
Brute-force	none	$O(S_q S_r)$

Table 1. Runtimes of approximate furthest neighbor algorithms.

DrusillaHash has a similar structure to the query-dependent approximate furthest neighbor algorithm of Pagh et al. [12] (“QDAFN”); except for three important differences: (i) the vectors v_i corresponding to each table are drawn using properties of the reference set, (ii) there is no priority queue structure when scanning the tables, and (iii) the projection bases chosen cannot be too similar. Although **DrusillaHash** can involve more setup time, our empirical simulations show it is able to provide better results with fewer hash tables and points in each hash table, resulting in better overall performance for a given level of approximation.

Table 1 gives a comparison of the runtimes of different approximate furthest neighbor algorithms. Note that **DrusillaHash** and QDAFN have the same asymptotic setup time for the same l and m ; but in practice, the overhead of **DrusillaHash** setup time is higher than QDAFN for equivalent l and m . But again it must be noted that to provide the same results accuracy, l and m may generally be set smaller with **DrusillaHash** than QDAFN.

6 Guaranteed approximation

Next, we wish to consider the problem of an absolute approximation guarantee: in what situations can we ensure that the furthest neighbor returned is an ϵ -approximate furthest neighbor?

Algorithm 2 **GuaranteedDrusillaHash**: guaranteed approximate k -furthest neighbor search.

```

1: Input: reference set  $S_r$ , query set  $S_q$ , number of neighbors  $k$ , acceptable approxi-
   mation level  $\epsilon$ , table size  $m$ 
2: Output: array of furthest neighbors  $N[]$ 

3: {Pre-processing: mean-center data.}
4:  $m \leftarrow \frac{1}{n} \sum_{p_r \in S_r} p_r$ 
5:  $S_r \leftarrow S_r - m$ ;  $S_q \leftarrow S_q - m$ 

6: {Pre-processing: build GuaranteedDrusillaHash tables.}
7:  $V \leftarrow \{\}$ 
8: for all  $p_r \in S_r$  do
9:    $n[p_r] \leftarrow \|p_r\|$  {Initialize norms of points.}
10:  $\delta \leftarrow \frac{\epsilon}{15}$ 
11: while  $\max_{p_r \in S_r} n[p_r] > \delta \max_{p_r \in S_r} \|p_r\|$  do
12:    $p_i \leftarrow \operatorname{argmax}_{p_r \in S_r} n[p_r]$  {Take next point with largest norm.}
13:    $v_i \leftarrow p_i / \|p_i\|$ 
14:    $V \leftarrow V \cup \{v_i\}$ 

15: {Calculate distortions and offsets.}
16: for all  $p_r \in S_r$  such that  $n[p_r] \neq 0$  do
17:    $O[p_r] \leftarrow p_r^T v_i$ 
18:    $D[p_r] \leftarrow \|p_r - O[p_r]v_i\|$ 
19:    $s[p_r] \leftarrow |O[p_r]| - D[p_r]$ 

20: {Collect points that are well-represented by  $p_i$ .}
21:  $R_i \leftarrow$  points corresponding to largest  $m$  elements of  $s[\cdot]$ 
22: for all  $p_r \in R_i$  do
23:    $n[p_r] = 0$  {Mark point as used.}

24: {Set shrug point (if we can).}
25: if there is any point such that  $n[p_r] \neq 0$  then
26:    $p_{sh} \leftarrow$  some point such that  $n[p_r] \neq 0$ 
27: else
28:    $p_{sh} \leftarrow \emptyset$ 

29: {Search for furthest neighbors.}
30: for all  $p_q \in S_q$  do
31:   for all  $R_i \in R$  do
32:     for all  $p_r \in R_i$  do
33:       if  $d(p_q, p_r) > N_k[p_q]$  then
34:         update results  $N[p_q]$  for  $p_q$  with  $p_r$ 
35:       if  $p_{sh} \neq \emptyset$  and  $d(p_q, p_{sh}) > N_k[p_q]$  then
36:         update results  $N[p_q]$  for  $p_q$  with  $p_{sh}$ 

```

It turns out that this is possible with a modification of **DrusillaHash**, given in Algorithm 2 as **GuaranteedDrusillaHash**. This algorithm, instead of taking a number of tables l , takes an acceptable approximation level ϵ . The parameter m does not affect the theoretical results, and would only be interesting as an implementation detail.

The algorithm is roughly the same as **DrusillaHash**, except for that more tables are added until all points with norm greater than $\delta \max_{p_r \in S_r} \|p_r\|$ are contained in some hash table, and an extra point called the *shrug point* is held. The shrug point is set to be any point within the small zero-centered ball of radius $\delta \max_{p_r \in S_r} \|p_r\|$. This is needed to catch situations where p_q is close to every point in R_i , and serves to provide a “good enough” result to satisfy the approximation guarantee.

Because **GuaranteedDrusillaHash** collects potentially huge numbers of hash tables that may contain most of the points in S_r , the algorithm is primarily of theoretical interest. Although the algorithm will outperform brute-force search as long as the hash tables do not contain nearly all of the points in S_r , it is not likely to be practical for large S_r ; thus, our interest in **GuaranteedDrusillaHash** is primarily theory-oriented.

With the algorithm introduced, we may present our theoretical result. First, we introduce a utility lemma.

Lemma 1. *Given a mean-centered set S_r and a query point p_q with true furthest neighbor p_{fn} , if $\|p_q\| < \frac{1}{3} \max_{p_r \in S_r} \|p_r\|$, then $\|p_{fn}\| > \frac{1}{3} \max_{p_r \in S_r} \|p_r\|$.*

Proof. This is a simple proof by contradiction: suppose $\|p_{fn}\| \leq \frac{1}{3} \max_{p_r \in S_r} \|p_r\|$. Then, the maximum possible distance between p_q and p_{fn} is bounded above as $d(p_q, p_{fn}) < \frac{2}{3} \max_{p_r \in S_r} \|p_r\|$. But the minimum possible distance between p_q and the largest point in S_r is bounded below as

$$d(p_q, \operatorname{argmax}_{p_r \in S_r} \|p_r\|) \geq \max_{p_r \in S_r} \|p_r\| - \frac{1}{3} \max_{p_r \in S_r} \|p_r\| = \frac{2}{3} \max_{p_r \in S_r} \|p_r\|. \quad (3)$$

This means that the largest point in S_r is a further neighbor than p_{fn} , which is a contradiction. \square

We may now prove the main result.

Theorem 1 *Given a set S_r and an approximation parameter $\epsilon < 1$ and any table size $m > 0$, **GuaranteedDrusillaHash** will return, for each query point p_q , a furthest neighbor \hat{p}_{fn} such that*

$$\frac{d(p_q, p_{fn})}{d(p_q, \hat{p}_{fn})} < 1 + \epsilon \quad (4)$$

where p_{fn} is the true furthest neighbor of p_q in S_r . That is, \hat{p}_{fn} is an ϵ -approximate furthest neighbor of p_q .

Proof. We know from Lemma 1 that if the norm of p_q is less than 1/3 of the maximum norm of any point in S_r , then the true furthest neighbor must have norm greater than 1/3 of the maximum norm of any point in S_r . Since δ is always less than 1/3 in Algorithm 2, we know that any such point will be contained in some hash table R_i , and thus the algorithm will return the exact furthest neighbor in this case.

The only other case to consider, then, is when the norm of the query point is large: $\|p_q\| \geq \frac{1}{3} \max_{p_r \in S_r} \|p_r\|$. But we already know due to the way the algorithm works, that if $\|p_{fn}\| \geq \delta \max_{p_r \in S_r} \|p_r\|$, then p_{fn} will be contained in some

hash table R_i and the algorithm will return p_{fn} , satisfying the approximation guarantee.

But what about when $\|p_{fn}\|$ is smaller? We must consider the case where $\|p_{fn}\| < \delta \max_{p_r \in S_r} \|p_r\|$. Here we may place an upper bound on the distance between the query point and its furthest neighbor:

$$d(p_q, p_{fn}) \leq \|p_q\| + \|p_{fn}\| < \|p_q\| + \delta \max_{p_r \in S_r} \|p_r\|. \quad (5)$$

We may also place a lower bound on the distance between the query point and its returned furthest neighbor using the shrug point p_{sh} . The distance between p_q and p_{sh} is easily lower bounded: $d(p_q, p_{sh}) \geq \|p_q\| - \delta \max_{p_r \in S_r} \|p_r\|$. This is also a lower bound on $d(p_q, \hat{p}_{fn})$. We may combine these bounds:

$$\frac{d(p_q, p_{fn})}{d(p_q, \hat{p}_{fn})} < \frac{\|p_q\| + \delta \max_{p_r \in S_r} \|p_r\|}{\|p_q\| - \delta \max_{p_r \in S_r} \|p_r\|}. \quad (6)$$

Now, define the convenience quantity α as

$$\alpha = \frac{\max_{p_r \in S_r} \|p_r\|}{\|p_q\|}. \quad (7)$$

Because of our assumptions on p_q , we know that $\alpha \leq 3$. This also means that $\alpha^2 \leq 3\alpha$. Similarly, we know that $\delta < 1$, which means that $\delta^2 < \delta$. Using these inequalities, we may further simplify Equation 6.

$$\frac{d(p_q, p_{fn})}{d(p_q, \hat{p}_{fn})} < \frac{1 + \delta\alpha}{1 - \delta\alpha} \quad (8)$$

$$= \frac{1 + 2\delta\alpha + \delta^2\alpha^2}{1 + \delta^2\alpha^2} \quad (9)$$

$$< 1 + 2\delta\alpha + \delta^2\alpha^2 \quad (10)$$

$$< 1 + 5\delta\alpha \quad (11)$$

and since $\alpha \leq 3$ and $\delta = \epsilon/15$, then it is true that

$$\frac{d(p_q, p_{fn})}{d(p_q, \hat{p}_{fn})} < 1 + \epsilon \quad (12)$$

and therefore the theorem holds. \square

Although **GuaranteedDrusillaHash** does not guarantee better search time than brute force under all conditions, it does in most conditions. As one example, consider a large dataset where the norms of points in the centered dataset are uniformly distributed. Some of these points will have norm less than $(\epsilon/15) \max_{p_r \in S_r} \|p_r\|$. These points (except the shrug point p_{sh}) will not be considered by the **GuaranteedDrusillaHash** algorithm, and this means that the **GuaranteedDrusillaHash** algorithm will inspect fewer points at search time than the brute-force algorithm.

Next, consider the extreme case, where there exists one outlier p_o with extremely large norm, such that the next largest point has norm smaller than

$(\epsilon/15)\|p_o\|$. Here, **GuaranteedDrusillaHash** with $m = 1$ will only need to inspect two points: the extreme outlier, and the shrug point p_{sh} .

On the other hand, there do exist cases where **GuaranteedDrusillaHash** gives no improvement over brute-force search, and every point must be inspected. If the dataset is such that all points have norm greater than $(\epsilon/15) \max_{p_r \in S_r} \|p_r\|$, then the tables R_i will contain every single point in the dataset.

These theoretical results show that it is possible to give a guaranteed ϵ -approximate furthest neighbor in less time than brute-force search, if the distribution of norms of S_r are not worst-case. But due to the algorithm’s storage requirement, it is not likely to perform well in practice and so we do not investigate its empirical performance.

7 Experiments

Next, we investigate the empirical performance of the **DrusillaHash** algorithm, comparing with brute-force search, query-dependent approximate furthest neighbor [12], and dual-tree exact furthest neighbor search as described by Curtin et al. [8] and implemented in **mlpack** [24]. Note that both brute-force search and the dual-tree algorithm return exact furthest neighbors; **DrusillaHash** and QDAFN return approximations.

We test the algorithms on a variety of datasets from the UCI dataset repository and **randu**, which is uniformly randomly distributed points. These datasets and their properties are listed in Table 2. In addition, hand-tuned parameters that produce $\epsilon = 0.05$ -approximate furthest neighbors (on average) are given for QDAFN and **DrusillaHash**.

The first experiment is to compare runtimes across all four algorithms. The approximate algorithms are tuned to return $\epsilon = 0.05$ -approximate furthest neighbors (using the parameters from Table 2). Table 3 shows the average runtimes of each of the four algorithms on each dataset across ten trials with the dataset randomly split into 30% query set, 70% reference set. I/O times are not included; the runtime only includes the time for the furthest neighbor search itself, including preprocessing time (building hash tables or building trees).

The **DrusillaHash** algorithm not only provides $\epsilon = 0.05$ -approximate furthest neighbors up to an order of magnitude faster than any other competing

Dataset	n	d	QDAFN params		DrusillaHash params	
			l	m	l	m
cloud	2048	10	30	60	2	1
isolet	7797	617	40	40	2	1
corel	37749	32	5	5	2	1
randu	100000	10	15	15	5	2
miniboone	130064	50	125	200	2	1
phy	150000	78	12	12	4	1
covertime	581012	55	15	20	6	2
pokerhand	1000000	10	15	50	50	8
susy	5000000	18	18	18	2	2
higgs	11000000	28	32	32	2	2

Table 2. Datasets and parameters.

Dataset	brute-force	dual-tree	QDAFN	DrusillaHash
cloud	0.0397s	0.0404s	0.010662s	0.0013302s
isolet	6.7535s	7.7057s	0.16485s	0.040634s
corel	10.292s	1.030s	0.021361s	0.021122s
randu	42.392s	28.004s	0.31600s	0.061855s
miniboone	187.26s	4.1047s	2.1648s	0.10362s
phy	370.06s	58.720s	0.20293s	0.18858s
covertypes	4077.9s	144.99s	1.2439s	0.20293s
pokerhand	–	852.00s	11.749s	8.0353s
susy	–	88.295s	21.678s	2.4467s
higgs	–	425.05s	56.094s	12.694s

Table 3. Runtimes for $\epsilon = 0.05$ -approximate furthest neighbor search.

algorithm, but it also needs to inspect fewer points to return an accurate approximate furthest neighbor (with the exception of the `pokerhand` dataset). In many cases, `DrusillaHash` only needs to inspect fewer than 10 points to find good furthest neighbor approximations, whereas QDAFN must inspect 50 or more.

Our datasets have two extreme examples: the `miniboone` dataset, which is high-dimensional but the data lies on a low-dimensional manifold, and the `randu` dataset, where points are uniformly distributed in the 10-dimensional unit ball.

For the `miniboone` dataset, `DrusillaHash` is able to easily recover only four points that provide average 1.05-approximate furthest neighbors. But because QDAFN chooses random projection bases, it takes very many to have a high probability of recovering good furthest neighbors. In our experiments, we were not able to achieve good approximation reliably until using as many as 125 projection bases. This effect was also observed with the `covertypes` dataset.

`DrusillaHash` also outperforms other approaches on the `randu` dataset, despite there being no structure for `DrusillaHash` to exploit. But the algorithm is still able to outperform others; this is because the algorithm specifically ensures that projection bases are not too similar (see line 22).

Another important property of `DrusillaHash` is that it gives a small maximum error compared to QDAFN. Figure 4 shows the maximum error of each approach as the number of points scanned increase on the `covertypes` dataset. For QDAFN, we have swept with $l = m$ from $l = 20$ to $l = 250$, and for `DrusillaHash`, we have set $m = l/3$ and swept l from 6 to 60.

Our experimental results have shown that `DrusillaHash` gives excellent approximation while only needing to scan few points. Whereas QDAFN seems to perform poorly in high-dimensional settings where the data lie on a low-

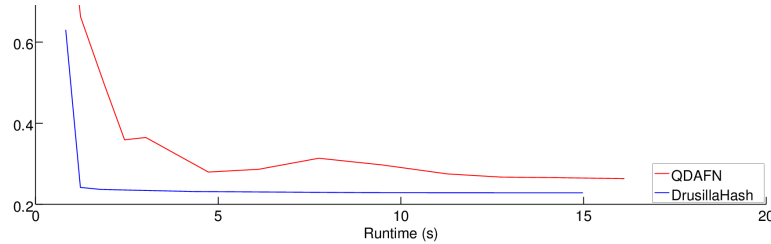


Fig. 4. Maximum error for `covertypes` dataset as a function of runtime.

dimensional manifold (because projection bases are random), **DrusillaHash** effectively captures the low-dimensional structure with few projection bases.

8 Conclusion

We have proposed an algorithm, **DrusillaHash**, that builds hash tables for approximate furthest neighbor search using the properties of the dataset to choose the projection bases. This algorithm design is motivated by our empirical analysis of the structure of the approximate furthest neighbor search problem, and the algorithm performs quite compellingly in practice. It scales better with dataset size than other techniques.

We have also proposed a variant, **GuaranteedDrusillaHash**, which is able to give an absolute approximation guarantee. This is a benefit that no other furthest neighbor hashing scheme is able to provide. However, this variant is not likely to be useful in practice.

Interesting future directions for this line of research may include combining a random projection approach with the approach outlined here. It would also be possible to generalize our approach to arbitrary distance metrics, including those where the points lie in an unrepresentable space. This could be done using techniques similar to some that have been used for max-kernel search [25,26].

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